Stability of Ferromagnetism in Hubbard models on two-dimensional line graphs

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Abstract

It is well known that the Hubbard model on a line graph has a flat band and ferromagnetic ground states in a certain density range. We show that for a Hubbard model on a line graph of a planar bipartite graph the ferromagnetic ground state is stable if one adds a special contribution to the kinetic energy which lifts the degeneracy of the lowest single particle state. Stability holds for sufficiently strong repulsion U. The model has extended single particle eigenstates, no degeneracy, and no band gap. It is therefore a good candidate for metallic ferromagnetism.

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1 Introduction and Results

Ferromagnetism in itinerant electron systems is an old and not yet fully understood problem in statistical physics. Kanamori [1] was the first to point out that the Hubbard model [2] is a good starting point for the investigation of ferromagnetism. It contains the two essential ingredients one needs to understand itinerant ferromagnetism: A single particle hopping term describing the motion of the electrons on a lattice and a purely local, repulsive interaction U between them.

The first major result towards ferromagnetism in the Hubbard model was the so called Theorem of Nagaoka [3, 4]. It states that for an infinite local repulsion and very close to a half filled band (one electron in addition to half filling) the ground state of the Hubbard model is fully polarized. The most general proof of this theorem was presented by Tasaki [5]. It uses a special basis for the multi-particle states in the Hilbert space and the Perron-Frobenius Theorem for matrices.

But the Theorem of Nagaoka describes the situation close to the singular point where the repulsive interaction is infinite and the band is half filled. In that case, each lattice site is occupied by one electron and one has a complete spin degeneracy, a pure paramagnet. Therefore, the Nagaoka Theorem is not a good starting point for a theory of ferromagnetism in the Hubbard model.

In 1989, Lieb [6] proved a result on the Hubbard model on bipartite lattices which yields a ferrimagnetic, not fully polarized ground state if the number of lattice sites in the two sublattices of the bipartite lattice is different and the difference is an extensive quantity. One can show that in this case the model has a purely dispersion-less or flat band and that there are other bands symmetrically above and below the flat band. Half filling means that the Fermi energy lies in the flat band, which means that the density of states at the Fermi level ρ_F is infinite.

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This result is in some sense complementary to the Nagaoka Theorem. The old criterion of Stoner for the occurrence of ferromagnetism, which is a simple mean-field result, states that $\rho_F U > 1$ for ferromagnetism to appear. Here U is the repulsive on-site interaction between electrons and ρ_F is the density of states per site at the Fermi level. This criterion over-estimates the occurrence of ferromagnetism. One knows examples of special lattices where even for $\rho_F = \infty$ and $U = \infty$ the ground state is not ferromagnetic. Nevertheless, an infinite value of ρ_F may be a good starting point for the study of ferromagnetism in the Hubbard model.

In 1991, the first example for a Hubbard model with $\rho_F = \infty$ was published which has a unique, fully polarized ferromagnetic ground state, the Hubbard model on the Kagomé lattice [7, 8]. This kind of ferromagnetism is called flat band ferromagnetism. It was shown to occur for a large class of lattices which are line graphs. Tasaki [9, 10] proved the existence of flat band ferromagnetism on another class of decorated lattices. Later on, a general criterion was derived which yields a necessary and sufficient condition for the uniqueness of the ferromagnetic ground state for a general situation where the hopping term in the Hubbard model has degenerate single-particle ground states [11, 12]. This result applies to any lattice with a lowest flat band, it applies even in a single band case with a partially flat band, but one needs a special lattice topology which is expressed as a criterion on the single-particle density matrix. Sekizawa [13] recently proved an extension of Tasaki's result for a general class of decorated lattices, which fulfill the criterion derived in [12].

Line graphs of planar bipartite graphs have special properties. The reason will become clear below. Using these special properties, we have been able to give a complete description of the ground states of the Hubbard model on this class of graphs in a certain density range [14]. Here we make use of these special properties as well.

Often, it was argued that the flatness of the band is artificial and that flat bands do not occur in nature. Another point is that in a flat band the Wannier states are single particle eigenstates of the Hamiltonian. The Fermi energy lies in a region where model has localized single-particle eigenstates. Although, due to the degeneracy, the distinction between localized and extended states is irrelevant, is is clear that arbitrary small local perturbations (point defects, line defects, disorder) favour localization. This means that in a realistic situation one probably has a ferromagnetic insulator and not a ferromagnetic metal. This argument does not apply to the case of a partially flat band, but even than the extensive degeneracy of the band is artifical.

Therefore, already in the beginning of the discussion of flat band ferromagnetism, Tasaki tried to show that the flat band ferromagnetism is stable if one introduces a small dispersion to the flat band and if the repulsion is sufficiently large. A first rigorous result in this direction was published in 1995 for a special class of decorated lattices where there is a gap between the flat band and the other bands [15, 16]. One year before, Kusakabe and Aoki published some numerical results that support the stability of flat band ferromagnetism on small lattices [17, 18]. Finally, in 2003, Tanaka and Ueda showed that even on the Kagomé lattice, which has no gap between the flat band and the next band, flat band ferromagnetism is stable if one adds a special hopping term to the Hamiltonian that yields a small dispersion in the formerly flat band [19].

All these examples indicate that at least for a large class of lattices flat band ferromagnetism may be stable: If one adds additional hopping terms to the Hamiltonian so that the flat band gets a dispersion, the ferromagnetic ground state remains the unique ground state for sufficiently large U. The present paper is a step in this direction.

Recently, Tamura et al proposed to study flat-band ferromagnetism experimentally using quantum dot super-lattices [20, 21]. They performed calculations for a Kagomé lattice within a tight-binding approximation for the quantum dot super-lattices, which includes a next nearest neighbour hopping term. The model was solved using exact diagonalization of small lattices. Although the next nearest neighbour hopping destroys the flat band, the result shows that flat band ferromagnetism can be observable in dot arrays.

Let us now summarize the results of the present paper:

Our results applies to a large class of graphs, line-graphs of planar, bipartite, two-connected graphs. It is the same class of graphs as in [14]. This class contains many two-dimensional lattices, but we do not need translational invariance. One property of the nearest-neighbour hopping on such graphs is that the lowest single-particle eigenstate is highly degenerate. The ground state of the full Hamiltonian for the case where the number of electrons equals the number of degenerate single-particle ground states is ferromagnetic and unique up to the usual spin degeneracy. We add a contribution to the kinetic energy which lifts the degeneracy. Then we are able to show that the ferromagnetic ground state remains the unique ground state of the system if the repulsive interaction U and the nearest-neighbour hopping t are sufficiently large.

The result of the present paper is a generalization of the result in [19] for the Kagomé lattice to a large class of lattices. In fact, the experimental realizations discussed in [20, 21] are line graphs of finite planar bipartite graphs. Furthermore, the additional hopping term contains many (local) parameters. And the result may be a good starting point for more general results in the future. For the Kagomé lattice, our proof is a simplification of the proof in [19].

The main difference between our result and the results obatined by Tasaki [15, 16] is that in our case there is no band gap between the lowest band and the higher bands. In addition, at least in the translational invariant case, the single particle eigenstates on our lattices are not localized. Localized single particle eigenstates or a gap in the single particle spectrum are criteria for a Mott or Anderson type of insulator. Therefore our class of graphs contains lattices which are good candidates for metallic ferromagnetism.

The rest of the paper is organized as follows. In the next section we introduce the notation, some definitions, the conditions we need, and we state the main result. We also give some comments on that result. The third section of the paper contains the proof.

2 Definitions and Results

As stated in the introduction, we investigate the Hubbard model on line graphs of planar bipartite graphs. Let us therefore introduce some definitions and properties concerning line graphs of planar bipartite graphs. We use some notions of standard graph theory which may be found in any text book on graph theory, see e.g. [22]. We use the notation in [14].

Let G be a bipartite planar 2-connected graph. $V(G)$ is the set of vertices, $E(G)$ the set of edges of G. Each edge $e \in E(G)$ connects two vertices $x, y \in V(G)$ and may be denoted as $e = \{x, y\}$. As in [14] we assume that G is 2-connected which means that no edge exists so that the graph decays into two unconnected subgraphs if this edge is deleted from G. A graph is bipartite if the vertex set V is a union of two disjoint vertex sets V_1 and V_2 so that each edge joins a vertex from V_1 to a vertex of V_2. In a bipartite graph, the length of each cycle is even.

A walk of length $n-1$ is a sequence $c = (x_1, e_1, x_2, e_2, \ldots, e_{n-1}, x_n)$. A path is a self avoiding walk, a cycle is a closed, self avoiding walk.

A planar graph can be represented in the plane as a set of point and lines between them so that there are no lines intersecting each other. The representation of the planar graph in the plane is called a plane graph. The representation is not necessarily unique. In the following we assume that the planar graph G is a plane graph. The results do not depend on the representation in the plane.

A plane graph divides the plane into a set of connected components, called faces. Most of the faces are bounded. Each plane graph has exactly one unbounded face. Let $F(G)$ be the set of bounded faces of G. Due to the famous Theorem of Euler, the number of bounded faces is $|F(G)| = |E(G)| - |V(G)| + 1$. We assume $|F(G)| > 1$. If there is no or only one bounded face, the results we want to show are trivial and uninteresting. The boundary of a face f is a cycle.

Let $L(G)$ be the line graph of G. The line graph of G is defined as follows: The vertex set of $L(G)$ is the set of edges $E(G)$ of the original graph. The vertices $e, e' \in E(G)$ are connected if

$|e \cap e'| = 1$, i.e. if the two edges of the original graph have a vertex in common. Note that a line graph of a plane graph is not necessarily a plane graph. The Kagomé lattice we mentioned above is the line graph of the hexagonal or honey-comb lattice. It is a plane graph. But the line graph of the square lattice is not planar.

Let $B = (b_{xe})_{x \in V(G),\, e \in E(G)}$ be the vertex-edge-incidence-matrix. $b_{xe} = 1$ if the vertex x belongs to the edge e, $b_{xe} = 0$ otherwise.

Let $\tilde{B} = (\tilde{b}_{fe})_{f \in F(G),\, e \in E(G)}$ be the face-edge-incidence-matrix. $\tilde{b}_{fe} = 1$ if the edge e belongs to the boundary of f, $\tilde{b}_{fe} = 0$ otherwise.

The number of edges of the boundary of f is $n_f = \sum_{e \in E(G)} \tilde{b}_{fe}$. Since the graph is bipartite, n_f is even.

Let $C = (c_{xf})_{x \in V(G),\, f \in F(G)}$ be the vertex-face-incidence-matrix. $c_{xf} = 1$ if the vertex x belongs to the boundary of f, $c_{xf} = 0$ otherwise. One has

$$c_{xf} = \frac{1}{2} \sum_{e \in E(G)} \tilde{b}_{fe} b_{xe} \tag{1}$$

We let $d_x = \sum_{f \in F(G)} c_{xf}$ and $D = \mathrm{diag}(d_x)$. d_x is the number of faces touching the vertex x.

Each face $f \in F(G)$ may be oriented. We choose a clockwise orientation. Each e may be oriented. Since G is bipartite, we choose the orientation of e such that it points from $V_1(G)$ to $V_2(G)$. We now introduce $S = (s_{fe})_{f \in F(G),\, e \in E(G)}$ where $s_{fe} = 1$ if e is part of the boundary of f and points into the direction of f, $s_{fe} = -1$ if e is part of the boundary of f and points into the opposite direction of f, $s_{fe} = 0$ otherwise.

A standard result in graph theory is $BS^t = 0$. Furthermore, the dimension of the kernel of B is $|E(G)| - |V(G)| + 1 = |F(G)|$. The columns of S^t form a basis of the kernel of B.

We now consider a Hubbard model on $L(G)$ with the Hamiltonian

$$H = \sum_{e,e' \in E(G),\sigma} t_{ee'} c^\dagger_{e\sigma} c_{e'\sigma} + \sum_{e \in E(G)} U_e n_{e\uparrow} n_{e\downarrow} \tag{2}$$

where

$$t_{ee'} = t \sum_x b_{xe} b_{xe'} - \sum_f \frac{s_f}{n_f} s_{fe} s_{fe'}. \tag{3}$$

We let $t > 0$, $s_f \geq 0$ and $U_e > 0$. $c^\dagger_{e\sigma}$ and $c_{e\sigma}$ are the usual creation and annihilation operators on the vertices of $L(G)$. $n_{e\sigma} = c^\dagger_{e\sigma} c_{e\sigma}$ is the number operator for electrons on e with the spin σ. $N = \sum_{e\sigma} n_{e\sigma}$ is the number of electrons. The first part of the Hamiltonian describes the hopping of electrons on $L(G)$, the second part is the local repulsive electron-electron interaction.

The first part of $t_{ee'}$ is the usual nearest neighbour hopping on $L(G)$ plus an additional term $2t\delta_{ee'}$. The lowest eigenvalue of $\sum_x b_{xe} b_{xe'}$ is zero. It's multiplicity is $|F(G)| = |E(G)| - |V(G)| + 1$. The second term lifts the degeneracy of this eigenvalue and does not change the other eigenvalues. Since the second part of the matrix $(t_{ee'})$ is negative semi-definite, all eigenvalues which are 0 for $s_f = 0$ become non-positive. For $s_f = 0$ this is the model discussed in [14].

The second part of the kinetic energy of the Hamiltonian can be written as $H_1 = -\sum_{f\sigma} s_f d^\dagger_{f\sigma} d_{f\sigma}$ where $d^\dagger_{f\sigma} = n_f^{-1/2} \sum_e s_{fe} c^\dagger_{e\sigma}$. Since the corresponding single particle states are not orthogonal, $\tilde{s}_{ff'} = [d_{f'\sigma}, d^\dagger_{f\sigma}]_+ = (n_f n_{f'})^{-1/2} \sum_e s_{fe} s_{f'e}$ is not diagonal.

Let $S_F = \mathrm{diag}(s_f)$ and $\tilde{S} = (\tilde{s}_{fg})_{f,g \in F(G)}$. Then single particle spectrum of H_1 is given by the spectrum of the matrix $-\sqrt{S_F}\tilde{S}\sqrt{S_F}$.

The Hubbard model has the usual $SU(2)$ spin symmetry. It commutes with the spin operators

$$S_z = \frac{1}{2}\sum_{e\in E(G)}(n_{e\uparrow}-n_{e\downarrow}) \quad (4)$$

$$S_+ = \sum_{e\in E(G)} c^\dagger_{e\uparrow}c_{e\downarrow} \quad (5)$$

$$S_- = \sum_{e\in E(G)} c^\dagger_{e\downarrow}c_{e\uparrow} \quad (6)$$

The eigenstates of H are eigenstates of $\vec{S}^2 = \frac{1}{2}(S_+S_- + S_-S_+) + S_z^2$ with eigenvalues $S(S+1)$ and S_z. Due to the $SU(2)$ symmetry, an eigenstate of H with a spin S is $(2S+1)$-fold degenerate, S_z takes values between $-S$ and S for the degenerate states.

Let us now state our main result:

Theorem: For sufficiently large $t > t_c$ and $U > U_c$ (both independent of the number of lattice sites and finite in the thermodynamic limit) and for $N = |F(G)|$ electrons, with G a 2-connected planar graph, the ground state of the Hubbard Hamiltonian (2) on the line graph $L(G)$ is fully polarized, $S = \frac{1}{2}N$, and unique up to the usual $(2S+1)$-fold spin degeneracy. In the subspace $S_z = S$ the unique ground state is $\prod_f d^\dagger_{f\uparrow}|0\rangle$ where $|0\rangle$ denotes the vacuum.

Before we start to prove this theorem, let us make some remarks:

(i) The ground state in the theorem is a fully polarized state. It's energy does not depend on U. This state is an eigenstate of the Hamiltonian for any value of U. But it is clear that it is not the ground state for $U = 0$. For $U = 0$ we obtain the ground state by filling the single particle eigenstates of H_1 successively with electrons with spins up and down. An exception occurs if a single particle eigenstate is degenerate, in that case Hund's rule applies. But generically, the degeneracy will not be of the order $|F(G)|$.

(ii) The proof of the theorem makes use of the fact that the columns of S^t form a basis of the kernel of B. In [14] we made use of this fact to completely describe all ground states of the Hamiltonian with $s_f = 0$ for $N \leq |F(G)|$. Now we use this property to prove a result for the ground state of H for $s_f \geq 0$ and $N = |F(G)|$. One might expect that it should be possible to extend this result to $N < |F(G)|$. But this is much harder. Even if $s_f = s$ for all $f \in F(G)$, a simple generalization of the theorem is not possible. The reason is that we use $H \geq -\sum_f s_f$ for sufficiently large U and t together with the fact that the ferromagnetic state $\prod_f d^\dagger_{f\uparrow}|0\rangle$ has the energy $-\sum_f s_f$. For $N < |F(G)|$ a generalization is difficult, since the proof uses the locality of the states $d^\dagger_{f\sigma}$. But the single particle ground states of H_1 are not local and therefore it is not possible to express the ferromagnetic eigenstates of H with lowest energy by local operators.

(iii) Although the proof makes use of the locality of the operators $d^\dagger_{f\sigma}$, the single particle eigenstates of H are generically not localized. Esp. this is not the case if G is a translational invariant lattice and $s_f = s$. In that case the system is a good candidate for a ferromagnetic metal: There are no artifical degeneracies, the single particle eigenstates are extended states, not localized states, and the Fermi energy does not lie in a band gap.

(iv) The proof makes use of the fact that G is a plane graph. For arbitrary line graphs, the degeneracy of the single particle ground state is $|E| - |V| + 1$ if G is bipartite, as for the case of a plane graph. One can even construct a basis using small cycles on G, similar to the boundaries of the faces of the plane graph. But the number small cycles is much larger than the number of single particle ground states. As a consequence, the bounds we shall use in the proof do not hold. Therefore, it is not possible to easily generalize the result to three dimensional lattices.

3 Proof

The Hamiltonian H can be written as a sum of local Hamiltonians $H = \sum_{f\in F(G)} H_f$ where

$$H_f = H_{f,1} + H_{f,2} + H_{f,3} \tag{7}$$

$$H_{f,1} = -\frac{s_f}{n_f} \sum_{e,e' \in E(G),\sigma} s_{fe} c^\dagger_{e\sigma} s_{fe'} c_{e'\sigma} \tag{8}$$

$$H_{f,2} = t \sum_{x \in V(G)} \frac{c_{xf}}{d_x} \sum_{e,e' \in E(G),\sigma} b_{xe} c^\dagger_{e\sigma} b_{xe'} c_{e'\sigma} \tag{9}$$

$$H_{f,3} = \sum_{x \in V(G)} \frac{c_{xf}}{2d_x} \sum_{e \in E(G)} b_{xe} U_e n_{e+} n_{e-} \tag{10}$$

Let us first discuss H_f. One has $H_f \geq -2s_f$. We will show that for sufficiently large t and U_e one obtains $H_f \geq -s_f$.

In a first step, we discuss H_f for $U_e = \infty$ and $t = \infty$. $H_{f,2} \geq 0$ and $t = \infty$ means that the single Hilbert space is restricted to single particle states with $H_{f,1}\phi = 0$. The single particle Hamiltonian $H_{f,2}$ is equivalent to the matrix

$$T_{f,2} = tB^t C_f D^{-1} C_f B \tag{11}$$

where $C_f = \mathrm{diag}(c_{xf})$ and $D = \mathrm{diag}(d_x)$ has been defined above. The kernel of $T_{f,2}$ is the kernel of $C_f B$.

In the following discussion we restrict ourselves to the subset of edges of $E(G)$ for which at least one matrix element of $T_{f,2}$ does not vanish. This subset consists of the edges of f and the edges connected to f. One can show that the dimension of the rank of $C_f B$ is $|f| - 1$ if no other edges are connected to f, $|f|$ otherwise. The first case has been excluded above since G must be 2-connected. This means that the dimension of the kernel of $C_f B$ is given by the number of edges connected to f but not an element of f. We call them outer edges of f. Their number is given by $r_f = \sum_{x \in f} d_{xf} - 2|f|$. Therefore we need to find r_f linear independent states that form a basis of the kernel of $C_f B$. The first state is $\phi_0(e) = s_{fe}$. The other basis states are constructed as follows: We choose e_0 to be one the outer edges of f. The other edges are numbered as $e_1, \ldots, e_{r_f - 1}$. We now let p_i be the path that starts at e_0, ends at e_i and runs clockwise around f. The path is oriented, it starts at e_0. If e_i is connected to the same vertex in f as e_0, it has length 2, i.e. it contains no edge of f. We let $\phi_i(e) = 1$ if e belongs to p_i and has the same orientation as p_i; $\phi_i(e) = -1$ if e belongs to p_i and has the opposite orientation; $\phi_i(e) = 0$ if e does not belong to p_i. Obviously, we have constructed r_f states. It is easy to see that each of these states belongs to the kernel of $C_f B$. Furthermore, there is at least one edge in f for which all ϕ_i vanish except ϕ_0. Since ϕ_i, $i > 0$ is the only state that does not vanish on e_i, the states ϕ_i are linearly independent. Thus, they form a basis of the kernel of $T_{f,2}$.

Now, we introduce

$$a^\dagger_{i\sigma} = \sum_e \phi_i(e) c^\dagger_{e\sigma} \tag{12}$$

One has $a^\dagger_{0\sigma} = d^\dagger_{f\sigma}$. Any multi-particle state which is an eigenstate of $H_{f,2}$ with eigenvalue 0 can be written as

$$\psi = \psi_0 + d^\dagger_{f\uparrow}\psi_+ + d^\dagger_{f\downarrow}\psi_- + d^\dagger_{f\uparrow} d^\dagger_{f\downarrow}\psi_1 \tag{13}$$

where $\psi_{0,\pm,1}$ are build by linear combinations of products of a suitable number of $a^\dagger_{i\sigma}$, $i > 0$ acting on the vacuum.

Now we use that $U = \infty$. This condition means that ψ has no double occupancy. We noted above that there exists one edge e for which all ϕ_i vanish except ϕ_0. Obviously, the last term in ψ has a double occupancy on this edge. Therefore, for $U = \infty$, ψ_1 must vanish.

Next, we want that ψ is a lowest energy eigenstate of $H_{f,1}$. Since $H_{f,1}\psi_{0,\pm,1} = 0$, we obtain $H_{f,1}\psi = -s_f\psi$ if and only if ψ_0 vanishes. Thus, for $U = \infty$ and $t = \infty$ one has $H_f \geq -s_f$ and the ground state of H_f is of the form

$$\psi = d^\dagger_{f\uparrow}\psi_+ + d^\dagger_{f\downarrow}\psi_- \tag{14}$$

By continuity, this result holds for sufficiently large but finite U and t as well, i.e. for $U > U_{cf}$ and $t > t_{cf}$. U_{cf} and t_{cf} are finite numbers and do not tend to infinity when G becomes large, as long as f remains finite. If e.g. G is some part of an infinite lattice, U_{cf} and t_{cf} do not change when one takes the thermodynamic limit.

As a consequence of the above result one has $H \geq -\sum_{f \in F(G)} s_f$.

Let us now consider the fully polarized state

$$\psi_{0\uparrow} = \prod_{f \in F(G)} d^\dagger_{f\uparrow} |0\rangle \tag{15}$$

The operator $\tilde{d}_{g\sigma} = \sum_f (\tilde{S}^{-1})_{gf} d_{f\sigma}$ is the dual operator to $d^\dagger_{f\sigma}$; we have $[\tilde{d}_{g\sigma}, d^\dagger_{f\sigma}] = \delta_{fg}$. We now obtain

$$\begin{aligned} H\psi_{0\uparrow} &= -\sum_f \frac{s_f}{n_f} d^\dagger_{f\uparrow} d_{f+\uparrow} \psi_{0\uparrow} && (16)\\ &= -\sum_{f,g} \frac{s_f}{n_f} \tilde{s}_{fg} d^\dagger_{f\uparrow} \tilde{d}_{g\uparrow} \psi_{0\uparrow} && (17)\\ &= -\sum_f \frac{s_f}{n_f} \tilde{s}_{ff} \psi_{0\uparrow} && (18)\\ &= -\sum_f s_f \psi_{0\uparrow} && (19) \end{aligned}$$

This shows that for sufficiently large values of t and U_e the fully polarized state ψ_{0+} is a ground state of H. The uniqueness of ψ_{0+} can be shown quite easily. In fact, we proved the uniqueness in [14] for $s_f = 0$. This proof can be carried over without any changes and it is not necessary to repeat it here.

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